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LCA FOR ENERGY SYSTEMS AND FOOD PRODUCTS

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Leveraging life cycle assessment and simplex lattice design in optimizing fossil fuel blends for sustainable desalination

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Abstract

Purpose This study aims to minimize the environmental impacts of thermal seawater desalination by optimizing the required fossil fuel mixture. Life cycle assessment (LCA) is applied to simulate the environmental impacts for each fuel mixture. To prevent mixture designs inherited collinearly from correlating LCA results, fuel mixtures are first sampled prior to conducting LCA and then later optimized using a regression-based methodology to reduce entailed environmental impacts.

Method Setting the functional unit to 1 m^3 of desalinated water induces different reference flows of energy requirements depending on the fuels used. Increasing the level of any fuel type within the fuel mixture scenario will cause a decrease in the level of the other fuel type(s) included. An augmented simplex lattice mixture (ASLM) design is applied to indicate correct experimental conditions and to prevent the correlation due to collinearity inherited from the nature of mixture problems. Regression models are formulated to represent life cycle impact assessment (LCIA) results in a closed form suitable for response surface methodology (RSM) optimization. An overall composite sustainability index (CSI) is a single index calculated by aggregating and normalizing corresponding LCIA responses of different units, ranges, and scales using the geometric mean-based method.

Results and discussion The results indicate that marine sediment ecotoxicity (MSE) is the category most adversely affected by multistage flash distillation (MSF). On a nationwide scale, the LCA optimized results scored a 17% reduction in associated environmental impacts, which corresponds to a 4.2% reduction in the county's carbon footprint and a 62% reduction in MSE while incurring a minor retrofitting cost to desalination facilities.

Conclusions High MSE results due to excessive fossil fuel consumption/burning in MSF should gain as much attention as paid toward global warming potential. High MSE entails the risk of having heavy metals entering the food chain. On the other hand, the geometric mean approach is found to be an effective model to aggregate the LCIA results into a single index while avoiding the subjectivity of the value judgment used in LCIA weighting. This approach serves as a unit-free rescaling method that is robust to outliers or large values examined across different LCIA impacts.

Keywords Life cycle assessment (LCA) · Design of experiment · Mixture designs · Regression · Response surface methodology · Optimization · Weighting · Geometric mean · Multistage flash distillation (MSF) · Desalination

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1 Introduction

Achieving sustainability in water production is arguably one of the biggest challenges worldwide (Aleisa and Al-Shayji 2018; Zodrow et al. 2017). This challenge is at its peak in Kuwait and for the other countries of the Gulf Cooperation Council (GCC) (Abdalla et al. 2017; Roudi-Fahimi et al. 2002), as the average annual per capita water renewable sources have already reached the so-called chronic water scarcity line (< 500 m^3 per capita/yr) (Cisneros et al. 2008). The GCC countries rely mainly on expensive thermal seawater desalination, followed by extraction from nonrenewable groundwater resources, to satisfy their demand for water (Aleisa and Al-Zubari 2017). The abundance of fossil fuels at relatively low extraction costs has allowed the predominant desalination technology in the GCC to be a thermal one, namely, multistage flash distillation (MSF). Although mega contracts in the GCC have been signed to make the transition to membrane-based desalination (IRENA 2019; Kaya et al. 2019; Ventures ONSITE 2019), MSF is still the leading technology due to its long running times between cleanings (6–24 months) and robustness to distilling feed water turbidity and salinity (Aleisa and Al-Shayji 2018; Chen and Yip 2018; Dahdah and Mitsos 2014; Mannan et al. 2019; Moser et al. 2013). Hence, MSF is still applied in 78% of the desalination plants (DPs) in the GCC, compared to 53% worldwide (Kaya et al. 2019; Verdier 2011). Approximately 81% of the total desalination production worldwide using MSF is generated in the GCC alone (Ghaffour et al. 2014; Purnama et al. 2005), with an estimated total production capacity of 4.7 billion m^3/yr (GCC Secretariat General 2015). However, when the urban air quality continued to show clear signs of elevated levels of air pollution (Abdulraheem 2010; Aleisa et al. 2011; Darwish et al. 2009), only then was the sustainability of MSF desalination in the GCC reconsidered. One distressing consequence is that Kuwait and other neighboring countries of the GCC are ranked among the top five per capita carbon dioxide emitters worldwide (The World Bank Institute 2014). Consequently, the new GCC strategy reform commits to investing up to $100 billion in renewable energy projects over the coming two decades (Kuwait Times 2016), and the mid- and long-range development plans in “Kuwait 2035” include strategies that are consistent with the UN Sustainable Development Goals (SDGs), Goal No. 7, “Ensuring Environmental Sustainability” (Tortell and Al-Essa 2011; UNDP 2014). This robust funding indicates that the perceived development priority (Lior 2017) in the GCC is finally transitioning toward sustainability (Aleisa and Al-Shayji 2018; Aleisa and Al-Zubari 2017; IRENA 2019). Unfortunately, current technologies for seawater desalination using renewables are not yet commercially available to satisfy the urban demand on a large scale (Aleisa and Al-Shayji 2018; Antipova et al. 2013). Only 1% of total desalinated water is currently based on energy from renewable sources (Ghaffour et al. 2014). A study conducted by Alkaisi et al. (2017) indicates that the economic performance evaluation of renewable energy desalination systems and their comparison with conventional systems is not conclusive due to many varying factors. Today, the small number of DPs operating on renewables has a high capital cost, low efficiency, and low productivity, which make renewable systems currently uncompetitive with conventional ones. Another comprehensive review of the recent projects of desalination using renewables states that “Bringing together renewable energy and desalination has been discussed at length without a major breakthrough of a large-scale” (Freyberg 2018; Karagiannis and Soldatos 2008). The study of Freyberg (2018) reviewed major water centers to conclude that trials of desalination using renewables have been promising on a small scale and are still far from ready to satisfy the aggressive urbanized trends of water consumption. Experts predict that the transitional period to renewables in desalination will consist of mixing energy sources, i.e., fossil fuel, solar, and wind, and then gradually increasing the proportion of renewables as cleaner technologies mature (ARFREE 2018).

Until a breakthrough takes place to secure clean energy-sourced reliable potable water production technology, a considerable reduction in the desalination carbon footprint can be realized in the meantime. This study aims to minimize the environmental impacts of seawater desalination by optimizing the fossil fuel mixture. The life cycle assessment (LCA) is applied to simulate the environmental impacts for each design mixture.

The LCA has been requisitely applied to assess the environmental impact of desalination technologies. A comprehensive literature review on more than thirty desalination LCA studies since the 2000s is found in Zhou et al. (2014). They identified the main factors that desalination practitioners of the LCA need to consider to improve the consistency and quality of the results. Earlier LCA studies on desalination identified the main raw materials and energy and outputs including products, byproducts, and emissions to different compartments (Friedrich 2002). Raluy et al. (2004, 2005, 2006) applied the LCA to examine environmental cradle-to-grave consequences MSF, multieffect evaporation (MED), and reverse osmosis (RO) technologies. In all cases, they demonstrated that the environmental load associated with the operation stage is the highest (88.6–99%) compared to all other phases. Vince et al. (2008) developed an LCA-based tool to conduct systematic evaluation of the environmental performances in potable water supply projects, in which they supported the Raluy et al. (2004, 2005, 2006) results in showing that operation has the highest environmental burden in potable water production, while chemical production for coagulation and remineralization represents the second major contribution to impacts. Lyons et al. (2009) applied the LCA to compare the impact of water importation, reclamation, and seawater desalination. Muñoz et al. (2010) made a comparison with water production systems in Spain with an emphasis on the impacts on freshwater resources. For LCA with a focus on membrane desalination, Zhou et al. (2011) focused on the effect and choice of impact assessment method on the overall result. In a follow-up study, Zhou et al. (2013) quantified the aquatic ecotoxic potential of the brine disposal in desalination. Tarnacki et al. (2011) demonstrated the opportunity to use waste heat in membrane desalination. Hancock et al. (2012) also applied the LCA to differentiate between several membrane technologies, including forward osmosis operated in osmotic dilution and others. Using the LCA to assess renewable energy for desalination, Jijakli et al. (2012) compared solar still, photovoltaic, and truck transportation for RO desalination alternatives in off-grid areas. The environmental impact of solar-MED was also assessed in Alhaj and Al-Ghamdi (2019) in seven locations distributed across six continents. Tarpani et al. (2019) also conducted LCA on MED distillation for brackish water with high levels of metalloids in isolated locations. Biswas and Yek (2016) conducted LCA on three separate drinking water production options: groundwater treatment plant, surface water treatment plant, and seawater DP (electrodialysis) to develop strategies for reducing the carbon footprint. Based on the work of Friedrich (2002) and others, Goga (2016) also used the LCA to compare two water treatment membrane plants that use alternative feed sources, namely, seawater- and mine-affected water. On the other hand, Shahabi et al. (2014) and Heihsel et al. (2019) used the LCA to quantify supply/value chain contributions to the overall environmental impact associated with DPs. Due to the socioeconomic implications of desalination, Ibrahim et al. (2018) and others have also applied the LCA within the overall sustainability framework (Lior 2017), often using mathematical modeling (Aleisa and Al-Shayji 2018; Antipova et al. 2013; Ifaei and Yoo 2019). Another focus area for desalination and LCA was on technologies applied to desalinate seawater intake from the Arabian Gulf (Al-Kaabi and Mackey 2019; Al-Shayji and Aleisa 2018; Aleisa and Al-Shayji 2018; Alhaj and Al-Ghamdi 2019; Jijakli et al. 2012; Mannan et al. 2019). In Mannan et al. (2019), for instance, the LCA was used to quantify environmental burdens using the "Nexus" approach while varying the gain ratio of MSF desalination. Along these lines, the aim of this study is to apply the LCA to evaluate the environmental impact of different fossil fuel blends generated using a mixture design method to desalinate seawater using MSF and then to find the optimal mixture that minimizes impacts across the life cycle impact assessment indicators.

As in Khang et al. (2017), the parameters of the LCA are used in an experimental context, where they can simultaneously vary within a certain range to define a multidimensional design space formulated using the design of experiments (DoE) methodology (Montgomery 2013). Since the amount of energy required to desalinate 1 m^3 for a specific technology and water properties is preset, the fuel mixtures are best sampled and optimized using the mixture design methodology (Montgomery 2013; Smith 2005) as opposed to the typical DoE.

In addition, mixture design-based regression is applied to postulate system governing equations that establish a metamodel or "model of models" to act as a stand-alone simplified mockup for the LCA that can be expanded to predict the environmental impact indicators for different DPs to be utilized for system optimization. The concept of LCA metamodels has been discussed in the literature under the topics of LCA predictions (Huijbregts et al. 2006), streamlining (Hanes et al. 2013; Hunt et al. 1998; Olivetti et al. 2013; Tecchio et al. 2018), LCA meta-analysis (Berger and Finkbeiner 2011; Padey et al. 2012, 2013), and others (Birkved and Heijungs 2011; Gardezi et al. 2016). Metamodeling the LCA through regression has demonstrated great advantages in abstracting the time-consuming LCA model building (Padey et al. 2012, 2013), providing an approach for selecting proxy life cycle impact categories in streamlined LCA, factor screening (Hunt et al. 1998; Pascual-Gonzalez et al. 2015), and model simplification (Abanda et al. 2013; Birkved and Heijungs 2011; De Soete et al. 2014; Gardezi et al. 2016; Hanes et al. 2013) and better interpretation and correlation (Berger and Finkbeiner 2011; Grant et al. 2016; Park and Seo 2003). In addition, metamodeling of the LCA has opened pathways toward kriging (Moreau et al. 2012a) and optimization (Pascual-Gonzalez et al. 2015) and, as in the case at hand, toward merging models with existing enterprise resource planning data systems (De Soete et al. 2014), neural networks (Park and Seo 2003), sensitivity analysis (Groen et al. 2017; Khang et al. 2017; Padey et al. 2013), and stochastic models (Bendato et al. 2016; Levy et al. 2002; Moreau et al. 2012b). In this study, the regression-based metamodel is optimized using response surface methodology (RSM) tools (Cornell 2002). The results require minor plant retrofitting costs but have a considerable positive impact on the environment (Peñate and García-Rodríguez 2011) until the shift to renewables gradually takes place (Kuwait Times 2016). Our dependent variable is an environmental impact result, and the independent variables that define the design space are the mixture proportions.

1.1 Why use a mixture design for optimizing fuel mix LCA?

When using the LCA as an experimentation tool, a well-structured methodology is required to efficiently and accurately explore the design space to better describe and understand the underlying system. In this context, when setting the system output to a functional unit of 1 m^3 of desalinated water, the reference flows for each mixture scenario become collinearly dependent, because increasing the level of any fuel type will cause a decrease in the level of other fuel type(s) in the mix. Let x_i denote the proportions of the fossil fuel types i, which include natural gas (NG, $i = 1$), gas oil (GO, $i = 2$), heavy fuel (HF, $i = 3$), and crude oil (CR, $i = 4$). These variables represent the decision variables. The constraints of this problem are as follows:

$$\mathbf{0} \leq \boldsymbol{x}_i \leq \mathbf{1} \quad (\boldsymbol{i} = \mathbf{1}, \ldots, \mathbf{4}) \tag{1}$$

and

$$\sum_{i=1}^{4} \boldsymbol{x}_i = \mathbf{1} \tag{2}$$

Based on the above constraints, there is a potentially serious problem with applying the classic regression model, namely, violation of the independency of the input variables (Smith 2005). The regression model suffers from collinearity, as Eq. (2) implies that the knowledge of three input parameters fully determines the fourth. This means that using classical regression will produce invalid conclusions. Mixture designs (Cornell 2002) are particularly suitable for addressing the class of problems subject to the conditions in Eqs. (1) and (2) . Analysis and optimization techniques for the RSM can be readily applied to minimize the environmental impacts by identifying the best fossil fuel mix combination with respect to the identified LCIA indicators.

2 Materials and methods

The methodology for using a mixture design to conduct experiments using the LCA and optimize MSF desalination for four fuel components, namely, NG, GO, CR and HF, is illustrated in Fig. 1 and described in the following sections.

2.1 Goal and scope definition

Since the literature indicates that over 95% of GHGs are attributed to the energy consumption of the operational phase in MSF (Biswas 2009; Lyons et al. 2009; Raluy et al. 2004, 2006; Vince et al. 2008), in this study, we focus on reducing the impacts caused by this phase. The *goal* of this study is to apply the LCA to evaluate the environmental impact of different fossil fuel blends generated using a mixture design method to desalinate seawater using MSF and then to find the optimal mixture that minimizes the impacts across life cycle impact assessment indicators. The system *boundaries* are of a second order (Goedkoop et al. 2010), in which seawater intake, energy requirements, materials, and additives during operation are considered, while the capital goods are excluded, hence, cradle-to-gate minus capital goods. The functional unit consists of 1 m^3 of desalinated water produced for potable use. The reference flows will vary according to the calorific values of the fuel types in the fuel mixture for each scenario. The LCA follows the four stages outlined by ISO 14040/44 (ISO 14044 2006a, b): goal and scope definition, life cycle inventory (LCI) analysis, life cycle impact assessment (LCIA), and interpretation (Finkbeiner et al. 2006; Goedkoop et al. 2010).

2.2 The augmented simplex lattice mixture design

In its original form, the experimentation points for the simplex lattice mixture are $\binom{\boldsymbol{q}+\boldsymbol{r}-\mathbf{1}}{\boldsymbol{r}}$ equally spaced values from $\mathbf{0}$ to $\mathbf{1}$ (Gorman and Hinman 1962; Montgomery 2013; Scheffe 1963) based on the number of components, $\boldsymbol{q}$, and the degree of the design, $\boldsymbol{r}$:

$$\boldsymbol{x}_i \in \left\{ \mathbf{0}, \frac{\mathbf{1}}{\boldsymbol{r}}, \frac{\mathbf{2}}{\boldsymbol{r}}, \ldots, \mathbf{1} \right\} \quad (\boldsymbol{i} = \mathbf{1}, \ldots, \boldsymbol{q}) \tag{3}$$

Developed by Scheffé (1958), the augmented simplex lattice mixture (ASLM) design (Cornell 2002; Gorman and Hinman 1962; Scheffe 1963) allows for more information on the inner portion of the response surfaces, thus capturing results with higher accuracy. The augmentation adds $\boldsymbol{q}+\mathbf{1}$ additional complete blends – including all components – to those depicted in the classical lattice coordinates provided in Eq. (3); these include the overall centroid and additional points located halfway between the vertices and the overall centroids (aka axial check blends) (Smith 2005). Figure 2 visualizes the design points, i.e., the experimental conditions at which the responses are measured. In the ASLM, vertices represent pure blend mixtures (i.e., one fuel type only). The design used is of the third degree in ASLM ($\boldsymbol{r}=\mathbf{3}$) and contains blends of ($\boldsymbol{x}_1, \ldots, \boldsymbol{x}_4$), i.e., binary blends for each pair of fuels and ternary blends that are mixed equally. The additional points due to lattice augmentation on Eq. (3) are shown in the open circles of Fig. 2.

Thus, the number of experimental points is $\binom{q+r-1}{r} + q + 1$, resulting in 25 experiments or scenarios in the LCA context. Hence, the design is a $\{4, 3\}$ ASLM design for 4 components of a third degree.

2.3 Life cycle inventory (LCI) analysis

The amount of energy required to desalinate seawater using MSF varies in the literature (Ahmad 2002; Aleisa and Al-Shayji 2018; Lattemann and Höpner 2008; Mezher et al. 2011; Miller et al. 2015; Raluy et al. 2005, 2006; Vince et al. 2008). The energy and chemical values used in this study were averaged over 1 year of MSF operation for seawater intake from the northern part of the Arabian Gulf, characterized by hyper-salinity of 45–57 ppt, a water temperature of 20–31 °C (John et al. 1990; Moser et al. 2013; Smith et al. 2007), and total suspended solids (TSS) of 14–29 mg/l (Al-

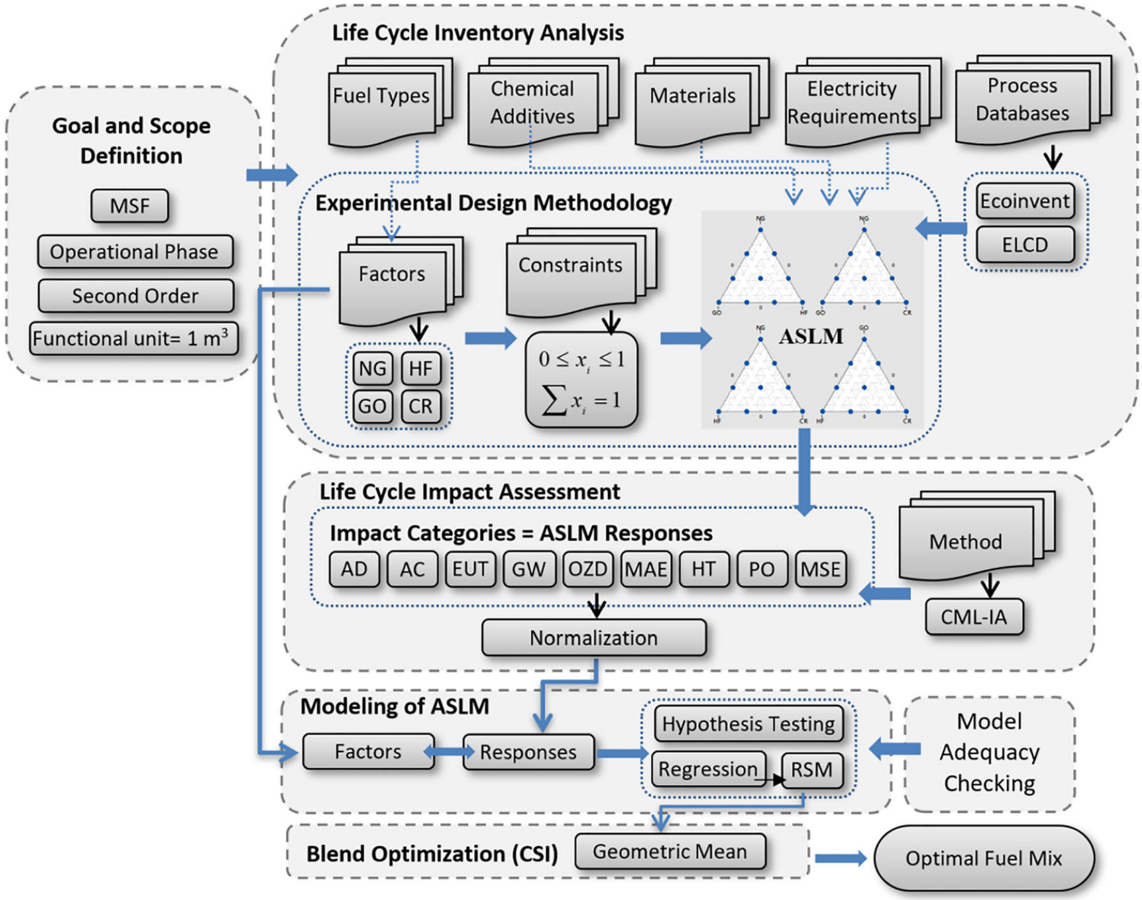

Fig. 1 Methodology for applying LCA and optimizing MSF desalination using four fuel components

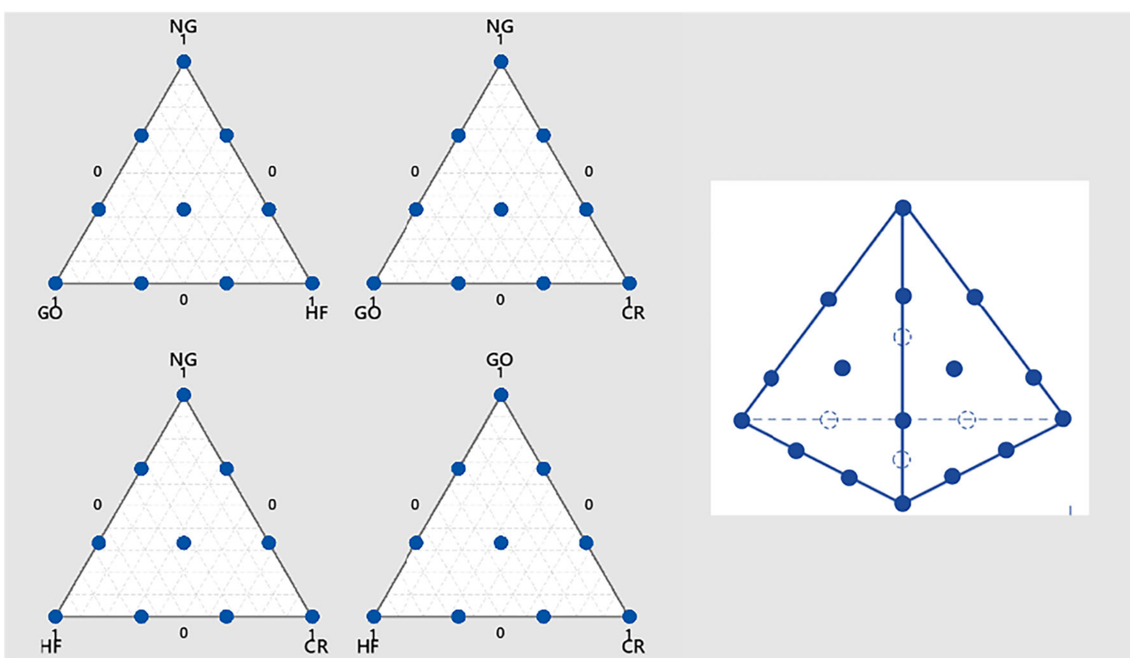

Fig. 2 The four faces of the tetrahedron of experimental conditions using the ASLM {4, 3} for four fuel components: NG (natural gas), GO (gas oil), CR (crude oil), and HF (heavy fuel)

Mutairi et al. 2014) in typical offshore intake areas. The MSF system efficiency has also been averaged over a year of operation across all MSF plant configurations in the country (MEW 2018). Thus, the functional unit required is 80 kWh/m^3 (Al-Shayji and Aleisa 2018; IRENA 2019; Mezher et al. 2011). The reference flow is a quantification of the amount of fuel required to deliver the BTU (British thermal unit) in the form of thermal energy described by the functional unit, which varies according to the heat content expressed by the net calorific value per barrel depending on the fossil fuel (Al-Shayji and Aleisa 2018) (see Appendix 1, Table 5). Since no change in the infrastructure (or gain ratio) is required, expressing the functional unit with respect to desalinated water or generated electricity, become two sides of the same coin. Let ρ_i denote the energy density per fossil fuel type i expressed in kWh/kg. Let ω_i indicate the required amount (kg) of each fossil fuel type i to produce 1 m^3 of desalinated water using the proportion, x_i; then, ω_i is estimated by $80x_i/\rho_i$ given the 80 kWh/m^3 needed to achieve our functional unit. Table 1 shows the mixtures (scenarios), proportions, and reference flow amounts for each scenario z (=1, …, 25) needed to desalinate 1 m^3 of seawater (the functional unit) using MSF for experimental points generated using the ASLM design (Eqs. (1)–(3)). For instance, blend $z = 12$ consists of 67% GO ($x_2 = 0.67$) and 33% HF ($x_3 = 0.33$) (see Table 1). A mixture of this proportion will require the following reference flow, namely, $\omega_1 = 0$, $\omega_2 = 4.92 = (80\ kWh)(0.67)/(11.8\ kWh/kg)$, $\omega_3 = 2.25 = (80kWh)(0.33)/(10.8\ kWh/kg)$, and $\omega_4 = 0$, to achieve desalination of the functional unit using MSF. These results are shown in 12th row of Table 1. Each blend is used as a notion of an “energy mix” supplied to MSF boilers and fed one fuel type at a time to satisfy the indicated proportions to desalinate seawater over a specific time period. The electrical energy required for MSF was set at 4 kWh/m^3. The local electricity generation mix, as a partial energy requirement, and the desalination chemical additives (see Table 2) were obtained from Al-Shayji and Aleisa (2018). The electricity required for desalination was obtained by creating a new electricity mix process based on Kuwait average data for 2016. The electricity mix is assumed to be fixed for all scenarios (blends) and thus is not altered as the fuel mixture proportions change. The LCI processes were obtained from the ecoinvent database v.2 (ecoinvent 2007) and adapted from the European Reference Life Cycle Database (ELCD) (JRC 2006).

Table 1 Mixture compositions used to desalinate 1 m^3 of seawater using MSF for experimental points generated using an ASLM displayed in proportions (x_i) and amounts (ω_i) in kg

Blend (scenario) z	Proportion				Mass reference flow (kg)			
	NG x_1	GO x_2	HF x_3	CR x_4	NG ω_1	GO ω_2	HF ω_3	CR ω_4
1	1.00	0	0	0	6.92	0	0	0
2	0.67	0.33	0	0	4.62	2.46	0	0
3	0.67	0	0.33	0	4.62	0	2.25	0
4	0.67	0	0	0.33	4.62	0	0	2.04
5	0.33	0.67	0	0	2.31	4.92	0	0
6	0.33	0.33	0.33	0	2.31	2.46	2.25	0
7	0.33	0.33	0	0.33	2.31	2.46	0	2.04
8	0.33	0	0.67	0	2.31	0	4.51	0
9	0.33	0	0.33	0.33	2.31	0	2.25	2.04
10	0.33	0	0	0.67	2.31	0	0	4.08
11	0	1.00	0	0	0	7.38	0	0
12	0	0.67	0.33	0	0	4.92	2.25	0
13	0	0.67	0	0.33	0	4.92	0	2.04
14	0	0.33	0.67	0	0	2.46	4.51	0
15	0	0.33	0.33	0.33	0	2.46	2.25	2.04
16	0	0.33	0	0.67	0	2.46	0	4.08
17	0	0	1.00	0	0	0	6.76	0
18	0	0	0.67	0.33	0	0	4.51	2.04
19	0	0	0.33	0.67	0	0	2.25	4.08
20	0	0	0	1.00	0	0	0	6.12
21	0.25	0.25	0.25	0.25	1.73	1.85	1.69	1.53
22	0.63	0.13	0.13	0.13	4.33	0.92	0.85	0.76
23	0.13	0.63	0.13	0.13	0.87	4.62	0.85	0.76
24	0.13	0.13	0.63	0.13	0.87	0.92	4.23	0.76
25	0.13	0.13	0.13	0.63	0.87	0.92	0.85	3.82

NG natural gas, *GO* gas oil, *HF* heavy fuel, *CR* crude oil

2.4 Life cycle impact assessment (LCIA)

The LCIA phase was performed according to CML-IA (Guinée et al. 2001) to calculate and compare the different fossil fuel blend responses for the points of the ASLM design. The impact categories shown in Table 3 were chosen to be relevant to the goal and scope of the study (Corporation and Curran 2006; Hauschild et al. 2017; ISO 14044 2006a, b). In addition, the selection of the impact categories was based on sector-specific studies (Chevalier et al. 2011) repeatedly examined in desalination LCAs, as depicted in the detailed review of Zhou et al. (2014) and others. The marine sediment ecotoxicity (MSE) is added to the common list, as the literature has indicated shoreline sediment distress (Dawoud 2012) and potential accumulation of heavy metals (Hoepner and Lattemann 2003; Lattemann and Höpner 2008). A normalization step (Guinée et al. 2001) was conducted to bring all LCIA results to the reference situation scores. This was done by dividing each score by the world total in 2000. Let y_{zq} denote the normalized score of mixture z (=1, …, 25) with respect to impact category q (=1, …, 9). The calculation of the magnitude of the category indicator results is performed for all mixtures/scenarios generated using the ASLM.

Table 2 MSF chemical additives per cubic meter of desalinated water (Al-Shayji and Aleisa 2018)

Chemical	Formula	Amount (g/m^3)	LCI materials in ecoinvent (ecoinvent 2007)
Sulfuric acid	H_2SO_4	7.33	Sulfuric acid
Antifoam	$C_3H_8O_2$	4.31E-01	Propylene glycol, liquid at plant
Anti-corrosion	Na_2SO_3	7.55	Sulfite inorganic chemical
Sodium nitrite	$NaNO_2$	1.33E-04	Nitro compounds, regional
Anti-scalant	H_3PO_4	2.52E-04	Phosphoric acid industrial grade 85% in H_2O
Cleaning	HCl	3.74E-03	Hydrochloric acid (30%) in H_2O
Neutralization: caustic soda	NaOH	3.02	Sodium hydroxide 50% in H_2O mix

2.5 Analysis of ASLM design

The ASLM design is conducted together with the regression models for each impact category using the fuel ingredients. The general regression formula is shown in Eq. (4).

$$\boldsymbol{y}_{zq} = \sum_{i=1}^{4} \boldsymbol{\beta}_{iq}\boldsymbol{x}_{zi} + \varepsilon_{zq} \quad (z = \mathbf{1}, \ldots, \mathbf{25}; q = \mathbf{1}, \ldots, \mathbf{9}) \tag{4}$$

β_{iq} denotes the theoretical regression coefficient that corresponds to the expected response from component i for each impact category, q (=1, …, 9). Its estimated value is denoted as $\hat{\beta}_{iq}$, and the estimates are found by standard regression techniques (see Eq. (4)). This depicts both the magnitude and direction of the association of a given response. ε denotes the random error term. The design was repeated for each impact category, q (=1, …, 9). In this setting, the null hypothesis, H_0, *indicates that there is no association between the term and the response*. Considering a significance level of 0.05 (α), $p \leq \alpha$ implies that there is a statistically significant association either *positively or negatively* with respect to each impact category. The regression models are then driven to create a simplified closed-form equation that constitutes an intermediate toward optimization. The regression models created can also be utilized to substitute modeling a separate LCA for different model parameters (i.e., different fossil fuel proportions) for desalination using MSF. In all generated regression models, the intercept term is not included in the regression models due to correlation (Smith 2005) imposed by Eq. (2).

Table 3 Impact categories evaluated at each experimentation point of the ASLM design

q	Impact category	Abbr.	Unit
1	Marine aquatic ecotoxicity	MAE	kg 1,4-DCB eq
2	Marine sediment ecotoxicity	MSE	kg 1,4-DCB eq
3	Global warming	GW	kg CO_2 eq
4	Human toxicity	HT	kg 1,4-DCB eq
5	Abiotic depletion	AD	kg Sb-eq
6	Acidification	AC	kg SO_2 eq
7	Eutrophication	EUT	kg PO_4^{3-} eq
8	Photochemical oxidation	PO	kg C_2H_4 eq
9	Ozone layer depletion	OZD	kg CFC-11 eq

2.6 Fuel blend optimization

The resultant normalized estimated multidimensional LCIA impact categories of each response $\hat{y}_q$ (for any design point, not just the 25 lattice points) are combined into a composite sustainability index (CSI), which corresponds to a *figure of merit* for the environmental impacts of the fuel mixtures (Aleisa and Al-Jarallah 2018; Aleisa and Al-Shayji 2018). Equation (5) defines the CSI for each mixture.

$$CSI = \sqrt[9]{\prod_{q=1}^{9} \hat{y}_q} \tag{5}$$

Compared to the arithmetic mean for the CSI (Aleisa and Al-Shayji 2018; Lior 2017; Zhou et al. 2012), the geometric mean can be applied when the aggregated items have different units and/or ranges. Thus, it serves as a unit-free rescaling method. The geometric mean is robust enough to avoid having the results dominated by outliers or large values examined across different LCIA responses. Smaller LCIA values indicate an overall environmentally cleaner mixture. Next, the CSI is numerically minimized by using an RSM optimization technique (Eq. (6)).

$$\begin{cases} \min CSI = \sqrt[9]{\prod_{q=1}^{9} \hat{y}_q} \\ \text{subject to } \hat{y}_q = \sum_{i=1}^{4} \hat{\beta}_{iq} x_i \ (\forall q) \\ \text{and } 0 \leq x_i \leq 1 \quad (\forall i) \\ \text{and } \sum_{i=1}^{4} x_i = 1 \end{cases} \tag{6}$$

Optimization of the geometric mean has long been used in finance and economics literature to optimize portfolio selection and maximize return on investment (James et al. 1977;

Latan et al. 1959; Latané and Tuttle 1967), where it is referred to as the mean compound return. It is a particularly useful measure for data that involve ratios, such as percentages (Clark-Carter 2005) or mixtures of ingredients, as in this case. Geometric means have the advantage of avoiding the use of weighting factors (WFs) when comprising a single index for LCA alternatives based on LCIA scores; these WFs are typically rendered as uncertain, subjective, and unreliable (ISO 14044 2006a, b; Pizzol et al. 2017; Tuomisto et al. 2012). The geometric mean optimization is conducted using the Minitab 18 software (Minitab 2018).

3 Results and analysis

3.1 LCA responses of the ASLM design blends

Both characterized and normalized environmental impacts are generated using CML-IA (V2.05 from the SimaPro software (PRé 2018)) for all scenarios/mixtures z (=1, …, 25) with respect to impact category q (=1, …, 9). Figure 3 presents the normalized LCIA results for the blends with the highest LCIA scores. It indicates that MSE is the category most adversely affected by MSF desalination, followed by MAE and AD. By tracing the results back to the LCI elements classified under the aforementioned impact categories, it was found that the excessive burning of fossil fuels in MSF causes an increase in AD, MAE, and MSE (Ozturk and Dincer 2019) impacts. Heavy metal (ions) from burning fossil fuel is often precipitated in the form of sulfides, which have very low solubility through precipitation and dissolution (Heijungs and Ligthat 2004). Heavy metals are transferred from the air compartment to the water column (MAE) and keep accumulating into the sediments (Hoepner and Lattemann 2003; Lattemann and Höpner 2008), hence the MSE high value. Within the MSE, blend/scenario $z = \{20\}$ of design point (0, 0, 0, 1), which indicates a vertex point of pure CR (see Table 1), scores the highest (worst), followed by $z = \{10\}$ of design point (0.33, 0, 0, 0.67), which is an edge point on the ASLM design that consists of two-thirds CR and one-third NG. For the MAE impact category, blend $z = \{20\}$ again has the highest performance. For AD, blend $z = \{7\}$ of design point (0.33, 0.33, 0, 0.33) scored the highest. The $z = \{7\}$ blend consists of equal proportions of NG, GO, and CR. The second worst blend with respect to AD is $z = \{1\}$, which is a pure blend of NG. The second worst blend contributing to AC is again $z = \{20, 10\}$. Equal proportions of NG, GO, and CR, $z = \{7\}$, contribute the most to GW.

3.2 ASLM analysis and regression

In this section, the analysis of the ASLM design is presented. Table 4 shows the $\hat{\beta}_{iq}$ for any term having $p \leq \alpha = 0.05$ and the $\hat{\beta}_{iq}$ for the main effects (pure blends) for all impact responses for producing 1 m^3 of desalinated seawater using MSF (see Eq. (4). Note that the p values cannot be calculated for the main effects due to the correlation imposed by Eq. (2). Across all impact indicators, interactions of NG*GO*CR and of NG*GO*HF*CR had $p \leq \alpha$, which resulted in a rejection of the null hypothesis, indicating a significant effect for all impact indicators. The negative estimated coefficient for the interaction NG*GO*CR indicates that the fuel components in the mixture act antagonistically. The squared coefficient of correlation, R^2, indicates how well the model fits the data. All the models have over 99% variance in the LCIA scores obtained, which indicates very good fits.

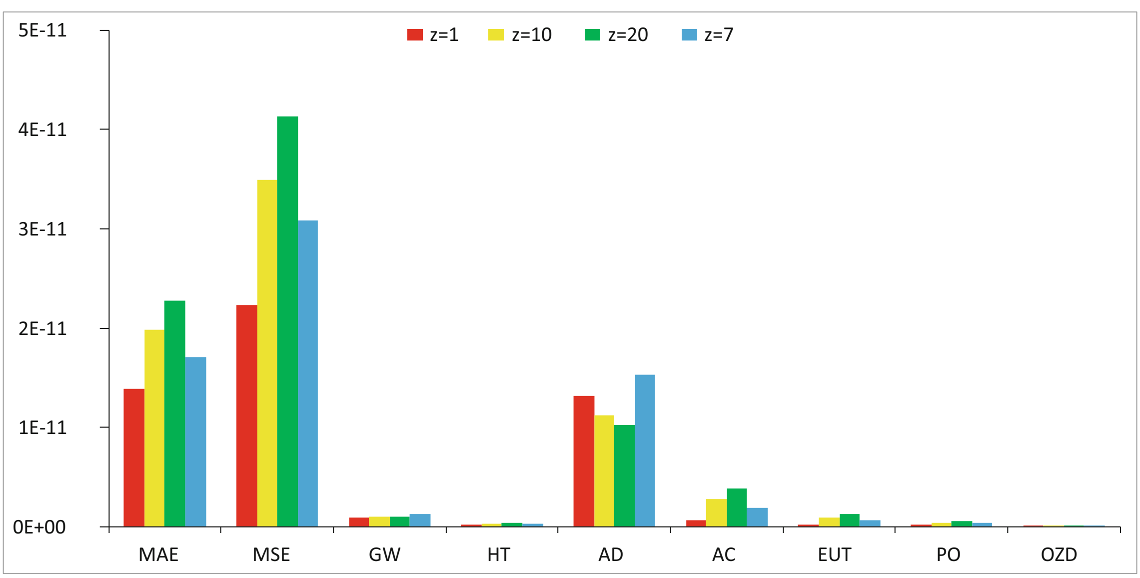

Fig. 3 The four simplex lattice design mixtures of fossil fuel blends that have the lowest normalized impact scores (person years)

Table 4 Estimated regression coefficients ($\hat{\beta}$) for responses obtained from the LCIA versus fuel mixtures identified for terms with $p \leq \alpha$ across all 25 mixtures (all binary mixtures had $p \geq \alpha$) in kg

q	Impact	Unit	NG	GO	HF	CR	NG*GO*CR	NG*GO*HF*CR	R^2(%)
1	MAE	kg 1,4-DCB eq	1570.3	881.9	806.6	2577.7	6768	− 30,715	99.94
2	MSE	kg 1,4-DCB eq	1251.1	624.7	570	1812.2	4798	− 21,773	98.49
3	GW	kg CO_2 eq	6.826	7.058	6.321	5.238	48.72	− 221.1	98.12
4	HT	kg 1,4-DCB eq	1.234	1.395	1.259	3.016	10.448	− 47.41	99.88
5	AD	kg Sb eq	0.195	0.176	0.161	0.152	1.376	− 6.24	97.82
6	AC	kg SO_2 eq	1.85E-02	1.70E-02	1.53E-02	1.04E-01	1.14E-01	− 5.16E-01	99.99
7	EUT	kg PO_4^{3-} eq	2.54E-03	4.03E-03	3.69E-03	1.59E-02	2.75E-02	− 1.25E-01	99.98
8	PO	kg C_2H_4 eq	1.35E-03	1.56E-03	1.42E-03	4.26E-03	1.16E-02	− 5.26E-02	99.94
9	OZD	kg CFC − 11 eq	7.00E-06	5.00E-06	4.00E-06	4.00E-06	3.70E-05	− 1.66E-04	99.53

The model errors (ε_{zq}) were assumed to be normally and independently distributed random variables with zero mean and constant variance σ_z^2. As a model validity check, all obtained βs were observed to have acceptable ranges of multicollinearity as indicated by the variance inflation factor (VIF): $VIF \leq 2.93$.

3.3 LCIA regression formulas using ASLM

This section presents the fit to mathematical equations to be used to model the LCIA response surfaces over the entire simplex space. The regression polynomials for the ASLM are derived in canonical form, where the number of terms in the polynomial is equal to that in the {4, 3} of the ASLM design.

Several types of regression models were investigated: linear, quadratic, cubic, and quartic, as well as other special forms of these. In this case, linear regression models represented a good fit (see Eq. (4)). Quartic regression models with the insignificant terms dropped ($p \leq \alpha$) also exhibited reasonable results, but the contribution to model accuracy was not justified. Therefore, the linear model is adopted, as it sufficiently captures most system variability. As an example, Eqs. (7) and (8) predict the expected LCIA values (in kg) for responses $q = 1$ and $q = 2$, respectively.

$$\hat{y}_{MAE} = 1570.3x_1 + 881.9x_2 + 806.6x_3 + 2577.7x_4 \qquad (7)$$

$$\hat{y}_{MSE} = 1251.1x_1 + 624.7x_2 + 570.0x_3 + 1812.2x_4 \qquad (8)$$

The remaining regression equations for q (=3, …, 9) can be derived similarly using the coefficients in Table 4. No intercept terms are included due to the correlation imposed by Eq. (2).

3.4 Response surfaces of LCIA using ASLM

The generated equations (see Eqs. (7) and (8)) can be interpreted graphically using the response contour plots (Fig. 4). Since the contour plots can show only three components at a time, NG, HF, and CR are examined, while GO is held constant at its minimum value (zero). These plots are useful in visualizing the location of the optimal design (minimum) and the direction in which the surface slope increases (or decreases) steeply. The Cox trace plots provided in Fig. 4 overlay the fitted regression functions of the four fossil fuel components for each LCIA impact category. Each equation term is varied from the low to the high value while keeping the remaining components at a constant centroid value. As expected, the MAE and MSE act analogously, since most substances that are important for the MAE are also important for the MSE (both rely on releases of ecotoxic chemicals). The MSE and MAE are both insensitive to NG and are the least adversely affected when increasing the HF and GO proportions and reducing CR. Likewise, HT, AC, EUT, and PO react analogously. The impacts are strongly adversely affected when increasing CR and reducing the remaining three fossil fuels. Despite the disparity in scale, the behaviors of GW, AD, and OZD are somewhat similar, with NG having a greater effect on OZD.

3.5 Optimal fossil fuel blend

As indicated in the methodology section (see Fig. 1), a numerical RSM optimization is conducted using Minitab 18. An important advantage for creating response surfaces for the LCA is the ability to optimize the derived functions either separately or collectively. Individual desirability, d, optimizes mixtures with respect to each separate response or impact category, q, according to Table 3, hence minimizing each impact individually.

The composite desirability, D, is calculated according to the CSI using Eqs. (5) and (6). This indicates how the mixture proportions optimize across all impact categories ($q = 1, \ldots, 9$) collectively. Figure 4 shows the optimization plot of individual desirability, d, and composite desirability, D. Overall, blend/scenario $z = \{17\}$ of design point (0, 0, 1, 0), which corresponds to a vertex

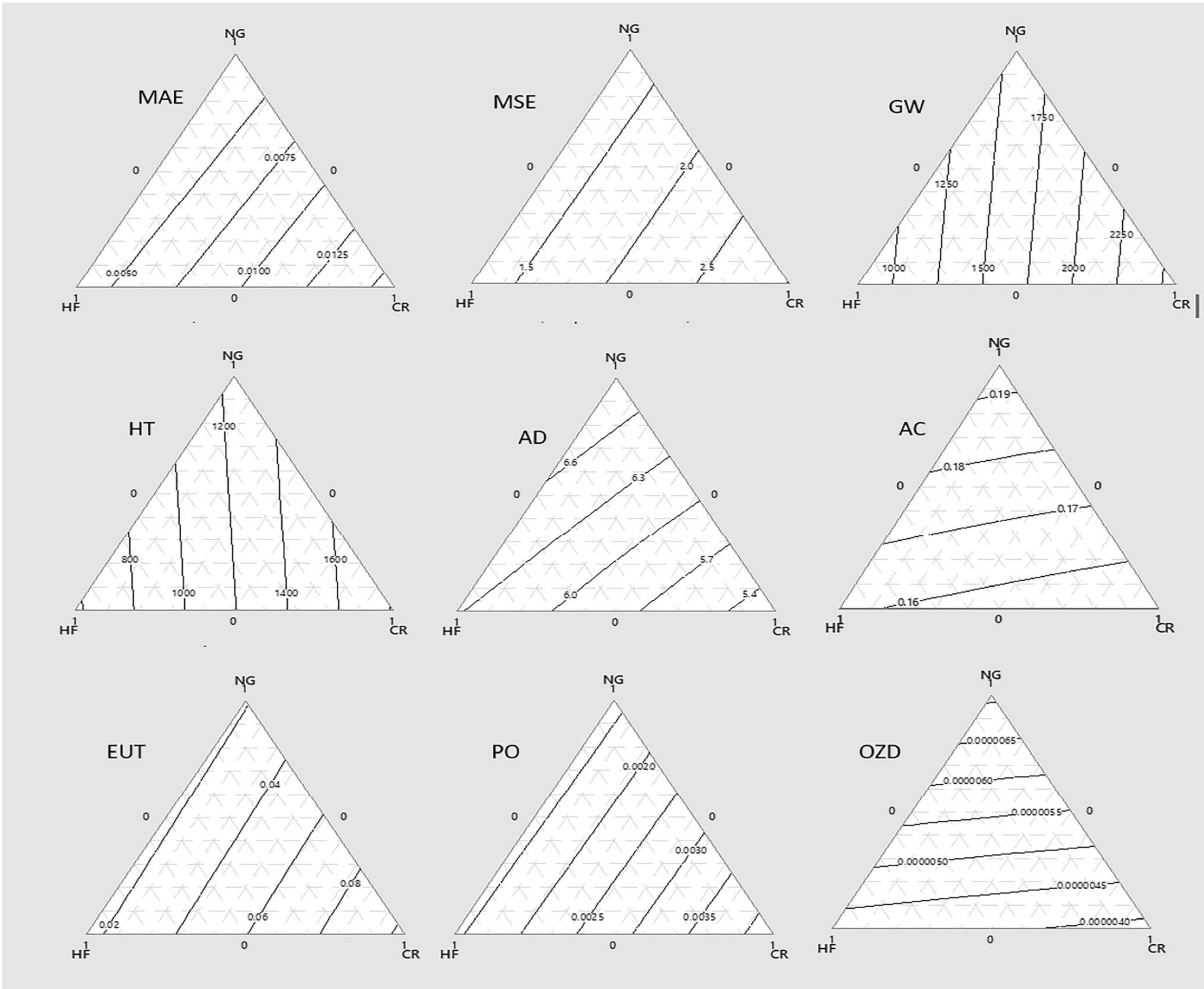

Fig. 4 Mixture contour plot for LCIA, with GO held constant at zero, shown in fossil fuel proportions to desalinate 1 m^3 of seawater, derived using regression equations

point of a pure blend of HF, scores the best (minimum) in CSI.

Figure 5 shows the results of CSI evaluation for all blends, ranked according to Eq. (5). Blend $z = \{17\}$ scores the best in terms of the CSI, followed by $z = \{14\}$ of design point (0, 0.33, 0.67, 0), which is an edge point on the ASLM design that consists of a binary blend of two-thirds HF and one-third GO. The third best blend is $z = \{12\}$, which is the counterpart blend of $z = \{14\}$; it consists of two-thirds GO and one-third HF (0, 0.67, 0.33, 0). On the other hand, the worst fuel blends according to the CSI are $z = \{20\}$, followed by $z = \{10\}$. Both of the $z = \{20, 10\}$ blends have the highest proportions of CR, with $z = \{20\}$ corresponding to pure CR (0, 0, 0, 1) and $z = \{10\}$ to two-thirds CR and one-third NG (0.33, 0, 0, 0.67).

4 Discussion

4.1 Implication of optimized results

The potential benefit of optimizing the fuel blend is a considerable reduction in associated environmental impacts. As shown in Fig. 6, for the current seven MSF DPs in Kuwait, a 17% reduction in the overall CSI (see Eq. (5)) can be achieved while incurring a minor retrofitting cost (Peñate and García-Rodríguez 2011). On a nationwide scale, this reduction is substantial, given that more than half of the oil production of the GCC countries is consumed by cogeneration for water and power DPs (Darwish et al. 2009; Fattouh and Mahadeva 2014; World Bank 2005). Characterized values of the optimized policy indicate that the carbon footprint of Kuwait DPs will reduce by 9.94%, which is equivalent to a

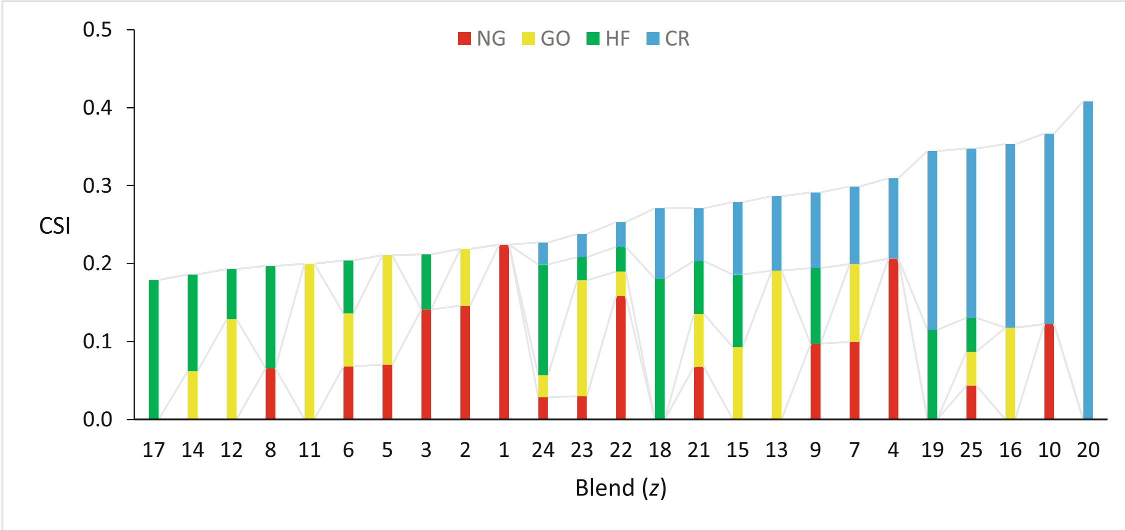

Fig. 5 Ranked CSI values for fossil fuel blends to desalinate 1 m^3 of seawater using MSF

reduction of 4.16 million tons annually based on baseline figures issued by Al-Mutairi et al. (2017).

In addition, it is important to note that the implications are more substantial on the electrical power generation side of the water/electricity cogeneration system, as electricity generation consumes over 60% of the fossil fuel required. It is important to note that shifting to the optimized policy requires neither crossover pipe changes nor changes in any intermediate or low pressure cylinders. This is because the ratio of power to water outputs is maintained by the design and included upfront. Hence, the optimized model can accommodate the demand and other technical considerations typical in MSF desalination planning (Dahdah and Mitsos 2014; Darwish et al. 2015; El-Nashar 2001; Ning 2015; Wu et al. 2013). More on the policy implications' note, Kuwait downstream oil refineries can support the required additional demand of HF for MSF desalination (KPC 2019; Paraskova 2019). HF is more economical to Kuwait than NG, since the latter has lower national reserve and thus is imported from neighboring countries for a higher price than the other fossil fuel types. The country also has plans to increase imports of NG as well (EXPORT.GOV 2018).

4.2 Marine sediment Ecotoxicity

The CO_2 reduction was considered as the baseline for the potential improvement because, first, of its contribution to climate change; second, CO_2 reduction is the main indicator in the national and regional environmental strategy; and third, it is considered in almost all desalination LCAs (Zhou et al. 2014), which allows for cross-validation (Chevalier et al. 2011) and comparison (Al-Kaabi and Mackey 2019; Alhaj and Al-Ghamdi 2019; Biswas 2009; Friedrich 2002; Hancock et al. 2012; Heihsel et al. 2019; Ibrahim et al. 2018; Jijakli et al. 2012; Mannan et al. 2019; Muñoz et al. 2010; Raluy et al. 2005; Shahabi et al. 2014; Tarpani et al. 2019; Vince et al. 2008; Zhou et al. 2011).

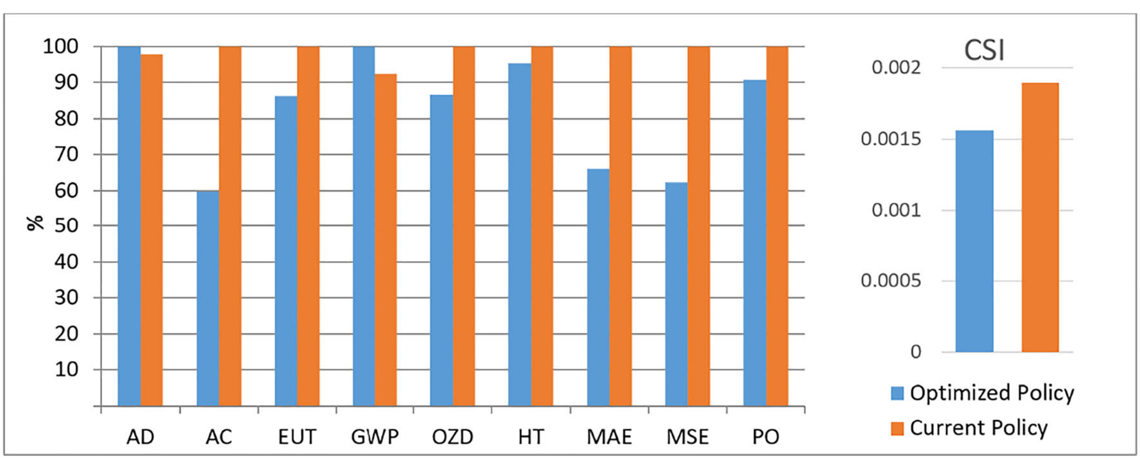

Fig. 6 Comparison between the current and optimized characterized environmental impacts for MSF desalination in Kuwait

Nevertheless, the normalized distress in the MAE and MSE due to excessive fossil fuel consumption in MSF desalination should gain similar attention. Contamination of heavy metals in sediment is regarded as a global crisis (Zohra and Habib 2016) that researchers have associated with desalination (Dawoud 2012; Hoepner and Lattemann 2003; Lattemann and Höpner 2008), oil refineries, and other industrial activities, with these heavy metal having found their way into the food chain in Kuwait (Al-Majed and Preston 2000; Bou-Olayan and Al-Yakoob 1994) and many other parts of the world (McDowell et al. 2004). Heavy metals such as cadmium, copper, iron, mercury, nickel, lead, zinc, and others (Zohra and Habib 2016) need to be investigated more in desalination LCA-associated contribution analysis. The reduction in MSE in the optimized policy is approximately 67%.

The brine disposal impact and aquatic ecotoxicity discussed in Muñoz et al. (2010), Meneses et al. (2010) and Zhou et al. (2013) also need to be considered. They were not incorporated in this study, as they are not yet part of the available LCIA methods.

4.3 Implication of geometric mean method

The geometric mean is a *novel* approach to LCIA single-index aggregation. It has roots in investment portfolio optimization. The geometric mean has the advantage of avoiding the subjectivity in value judgments conducted in the typical weighting of LCIA factors, which has been long criticized (ISO 14044 2006a, b; Pizzol et al. 2017; Tuomisto et al. 2012). While the optimization results appeared reasonable and were validated visually, it is important to alert the reader to some implication. The method is robust but is also unresponsive to changes that take place in relatively very high or low values in the different LCIA results. For instance, a 10% change in the MSE, say from 1570 to 141 in kg 1,4-dB eq, has the same effect on the geometric mean as a 10% change in OZD, say from 7.00E-06 to 6.30E-06 in kg CFC eq. In the optimization context, these extreme values could include a missed alternative optimal solution or even a global optimum. Although this disadvantage could be overcome when integrating the linear programming (LP) optimization into this problem, arguably, LP will also require a weighting for LCIA indicators that could bias the results in another way. Confirming global optima in this case will require additional inclusions of optimization theory and sensitivity analyses, an area to explore in future research on the metamodeling of LCA in general and that of MSF desalination.

5 Conclusions

In this study, the LCA was applied to evaluate the environmental impacts of using different fossil fuel blends to desalinate seawater via MSF in Kuwait. The generated blends of fuels were identified using the ASLM design to avoid the correlation inherent from the nature of the problem that would contaminate the analysis, particularly if classical regression was applied. The developed experimental design of LCA is of the third order, containing center and axial points to allow more information regarding the inner portion of the response surfaces. The LCI included seawater intake, energy requirements, materials, and additives during operation derived for each blend of the ASLM design. The LCIA results indicate that the MSE is the most adversely affected impact category by MSF desalination, followed by MAE, AD, and then AC.

ASLM analysis was used to derive the regression models used to construct the response surfaces. The LCIA responses obtained were adequately fitted to the linear regression models. The contour plots of the regression response surfaces were useful in visualizing the location of the optimal solution. Combined with Cox trace plots, visual inspection indicates that both the MSE and MAE are insensitive to NG and are least adversely affected when increasing the HF and GO proportions and reducing CR. Likewise, HT, AC, EUT, and PO react analogously. They are strongly adversely affected when increasing CR and reducing the remaining three fossil fuels. Despite the disparity in scale, the behaviors of GW, AD, and OZD are somewhat similar, with NG having a greater effect on OZD. The derived mathematical regression models were validated statistically as a stand-alone representation for LCA software, with 95% confidence. The postulated regression equations establish metamodels or “models of models” to act as stand-alone simplified mockups for the LCA, which can be expanded, allowing ample RSM optimization techniques and optimization, either separately or collectively, as well as making it possible to predict the environmental impact indicators for different desalination plants without the need to rerun the LCA software. For optimization, the normalized multidimensional LCIA responses for each blend were aggregated using a novel approach to LCA, which is based on the geometric mean. The geometric mean optimization has roots in portfolio investment optimization and is used in LCA to bypass the subjectivity inherited in typical LCIA weighting methods. Optimizing the CSI indicated that blend $z = \{17\}$ of design point $(0, 0, 1, 0)$, which corresponds to pure HF, scores the best (minimum) in terms of the CSI, followed by $z = \{14\}$ of design point $(0, 0.33, 0.67, 0)$, which is an edge point on the ASLM design triangle that consists of a binary blend of two-thirds HF and one-third GO. On the other hand, the worst fuel blends according to the CSI are $z = \{20\}$ and then $z = \{10\}$. Both blends $z = \{20, 10\}$ have the highest proportions of CR, with $z = \{20\}$ being pure CR and $z = \{10\}$ consisting of two-thirds CR and one-third NG. The realized benefit from this approach is a net 17% reduction in associated environmental impacts comprised and represented by the CSI. A 67% reduction in normalized MSE results, which could be realized through a reduction in heavy metals discounted by the optimized policy. On a nationwide scale, the 17% reduction is substantial, given that more than half of the oil production of the GCC countries is consumed by cogeneration of power and desalination plants (Darwish et al. 2009; Fattouh and Mahadeva 2014; World Bank 2005). This translates to a 9.94% reduction in carbon footprint for Kuwait desalination plants, which is equivalent to a reduction of 4.2% on the country level, with minimal cost of retrofication imposed. In addition, the downstream oil sector in Kuwait can accommodate the recommended policy shift demand-wise, economically and politically. Future research is directed toward creating a hybrid mixture of energies using fossil fuel and renewable energy sources coupled with RO and MED to pave the way toward shifting gradually to true sustainable water production on a large-scale.

Appendix 1

Table 5 Energy properties of NG, GO, HF, and CO to generate Kuwait electricity mix in kWh (Al-Shayji and Aleisa 2018)

Fuel (i)	Density @ 60F (MEW 1999)	Btu (MEW 1999)	Energy density kWh/kg (ρ_i)
NG	0.8729 (g/ml)	5.472E + 06 (Btu/bbl)	11.5546
GO	0.971 (g/ml)	5.707E + 06 (Btu/bbl)	10.8333
HF	0.846 (g/ml)	5.429E + 06 (Btu/bbl)	11.8284
CO	0.05 (lbs/SCF)	1012 (Btu/SCF)	13.0773

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